MPI on BG/L

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Outline

- Why MPI on BG/L?
- Challenges for MPI implementations provided by BG/L
- MPICH
  - The Abstract Device Approach to MPI implementation
  - MPICH-2 and scalability
  - Early results of IBM/Argonne Collaboration
- Scalable Process Management
  - MPD and the SciDAC Scalable Systems Software Project
  - MPI / Process Manager Interface
  - MPD and LoadLeveler on BG-L
  - Early results of IBM/Argonne Collaboration
- Conclusion
  - BG/L will provide at least one convenient and familiar programming and job scheduling environment

IBM Collaborators

- T. J. Watson
  - Jose Moreira
  - Gheorghe Almasi
  - Silvius Rus
- Haifa
  - Edi Shmueli
  - Yariv Aridor
  - Tamar Domany
  - Yosef Moatti

Why Have MPI on BG/L?

- BG/L does support MPI model
  - Separate address spaces (though small) for separate processes
- Vast number of parallel applications ready to run, or at least ready to begin work on
  - No barrier at programming model level (familiar message-passing model)
  - No barrier at language level (C, Fortran, C++, Fortran 90)
  - No barrier at communication library level (MPICH)
  - Memory requirement barriers likely at data/process level
  - Scalability barriers likely at algorithm level
- Demonstration of general purpose nature of machine
  - If MPI can be implemented, so can anything else

Challenges for an MPI Implementation on BG/L

- Small memory footprint (fingerprint?) per MPI process
- Scalability of data structures
  - Local size must be independent of total number of processes
  - Buffer management
- Scalability of algorithms
  - Must take advantage of BG/L hardware support, especially for collective operations
  - MPI topology routines will become more important
- Scalability of process manager interactions
  - Interaction with MPI library
  - Interaction with user
    - Convenient familiar direct interface to process manager (mpirun, mpiexec) or to batch scheduler (LoadLeveler)

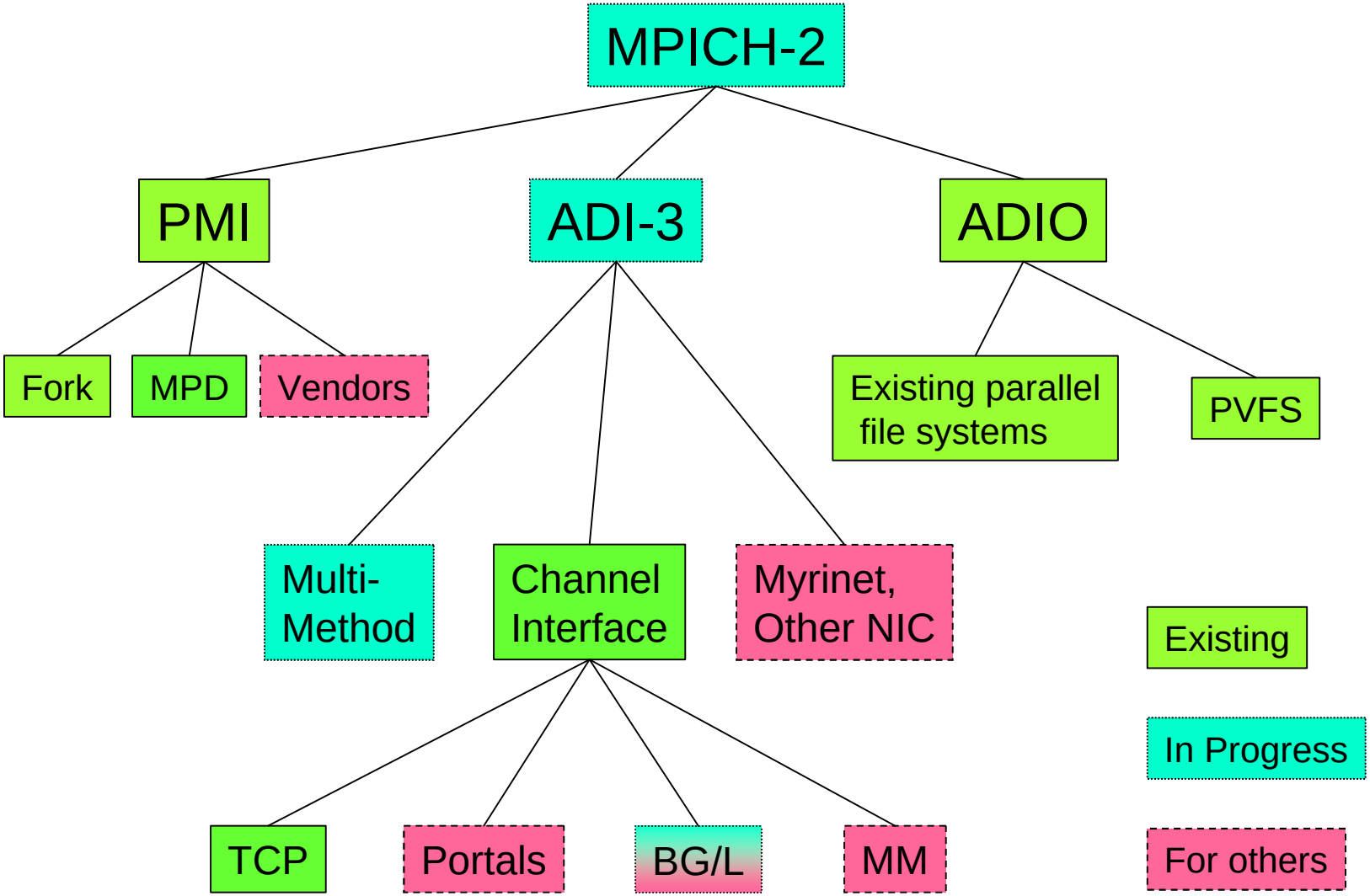
MPICH

- Goals
  - Supply research vehicle for MPI implementation issues
  - Promote standard programming model for users
  - Provide vendors and others with starting point for specialized MPI implementations (both commercial and research)
    - Architected to support replacement of components
- MPICH-1
  - Began during MPI standardization process
  - Current version 1.2.4, 2500 downloads/month
  - Complete implementation of MPI-1.2, plus I/O from MPI-2
  - Basis of many research and vendor implementations
    - MPICH-GM from Myrinet
    - MPI on ASCI Red (scalable to 3000+ nodes)
    - Early Cray, Meiko, SGI, HP/Compaq, NEC, other implementations
    - Research groups experimenting with lower levels
  - Windows version

MPICH-2

- Original goals of MPICH, plus
  - Scalability to 100,000 processes
  - Improved performance in multiple areas
  - Portability to new interconnects
  - Thread safety
  - Full MPI-2 Standard (I/O, RMA, dynamic processes, more)
- Not yet released
  - Detailed design complete and publicly available
  - Core functionality (point-to-point and collective operations) from MPI-1 complete
    - Early performance results
  - MPI-1 part to be released this fall

Structure of MPICH-2



The Abstract Device Interface

- Key to Performance and Portability
- MPICH-2 based on 3rd-generation ADI design (ADI-3)
- Research Topics
  - Combining performance with portability
  - Latency reduction
  - Multi-method
  - Thread safety
  - High-performance MPI datatype processing
  - Interaction with process management, MPI topology routines
  - Multiple approaches to collective operations
    - (For example, need not be in terms of point-to-point operations)
  - Sophisticated implementation of remote-memory operations
  - Dealing with faults

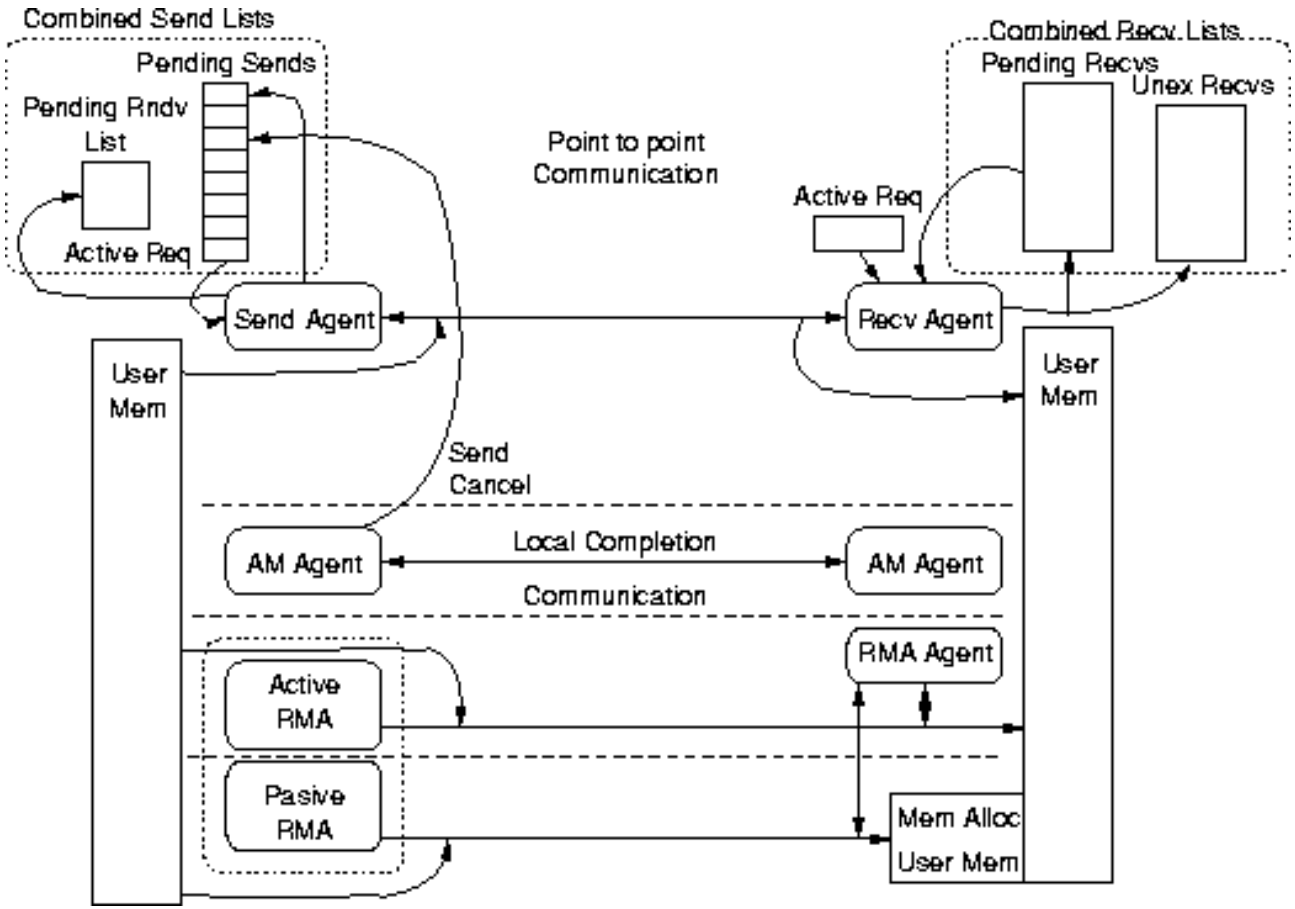
Possible Implementations of the ADI

- The “Channel” device
  - Small number of functions
  - Straightforward to implement
  - Sacrifices some opportunities for optimization
  - Current approach for BG/L
- The “Multimethod” device
  - Allows mixing of communication methods
    - TCP, Shared memory, NIC-based (Myrinet, Infiniband, others)
  - Made more difficult by MPI’s “ANY_SOURCE” in MPI_Recv
  - Intermethod interface by which new methods many be added
- The “Custom” device
  - Specialized to a particular environment
  - Usable by vendors (e.g., Myricom, who have studied ADI-3)
  - Optimum performance
  - Under discussion for BG/L

ADI Status and Plans

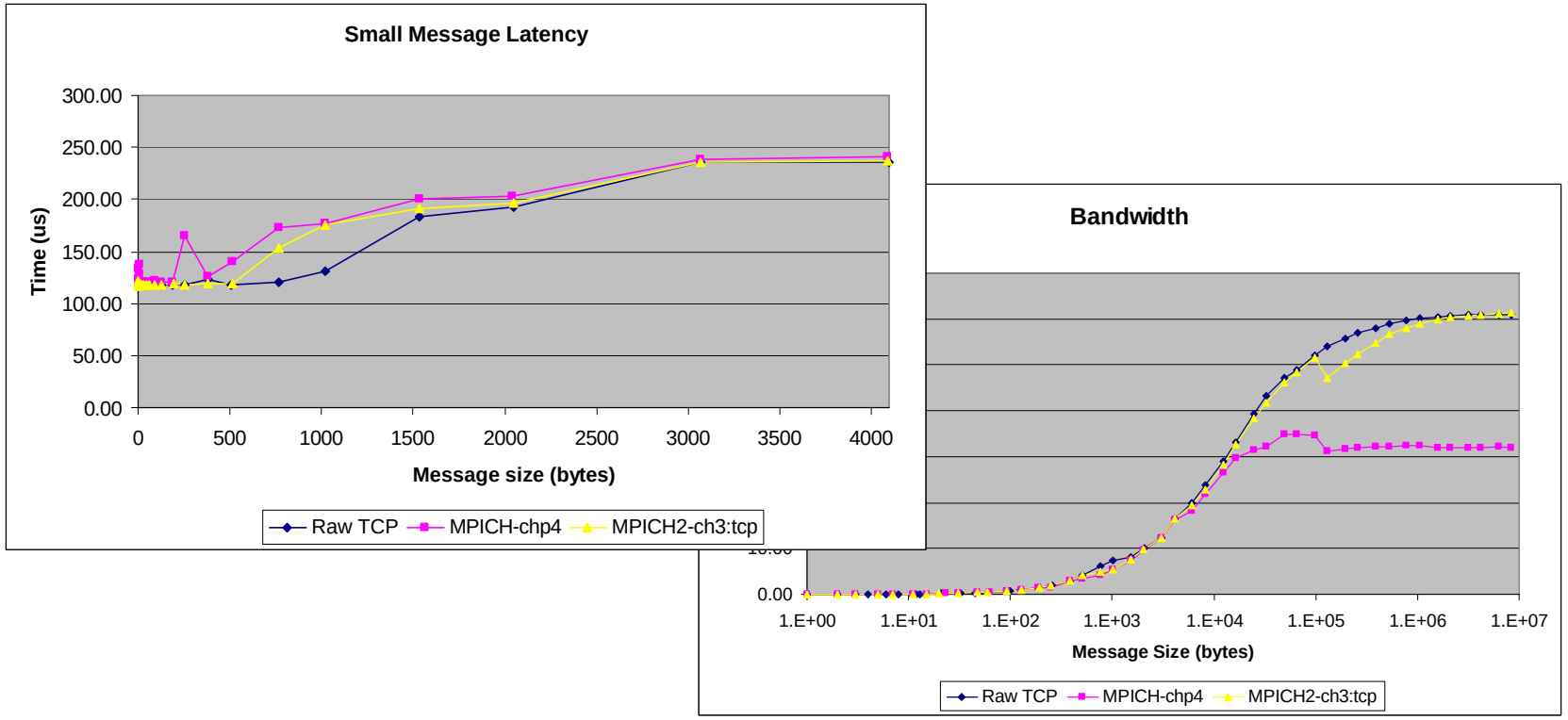
- Status
  - TCP implementation of the CH3 implementation of ADI-3 done
  - Multimethod implementation of ADI-3 under way
  - Both faster than in MPICH-1 (see following charts)
- Plans
  - Complete implementation of multimethod device
  - Tune and port to other environments (shared memory, Infiniband)
  - Continued vendor collaboration
    - Myricom plans to implement ADI-3
    - Current discussions with IBM on ADI/CH interface for BG/L
    - Collaborations with multiple Infiniband vendors in progress

An Example: CH3 Implementation over TCP



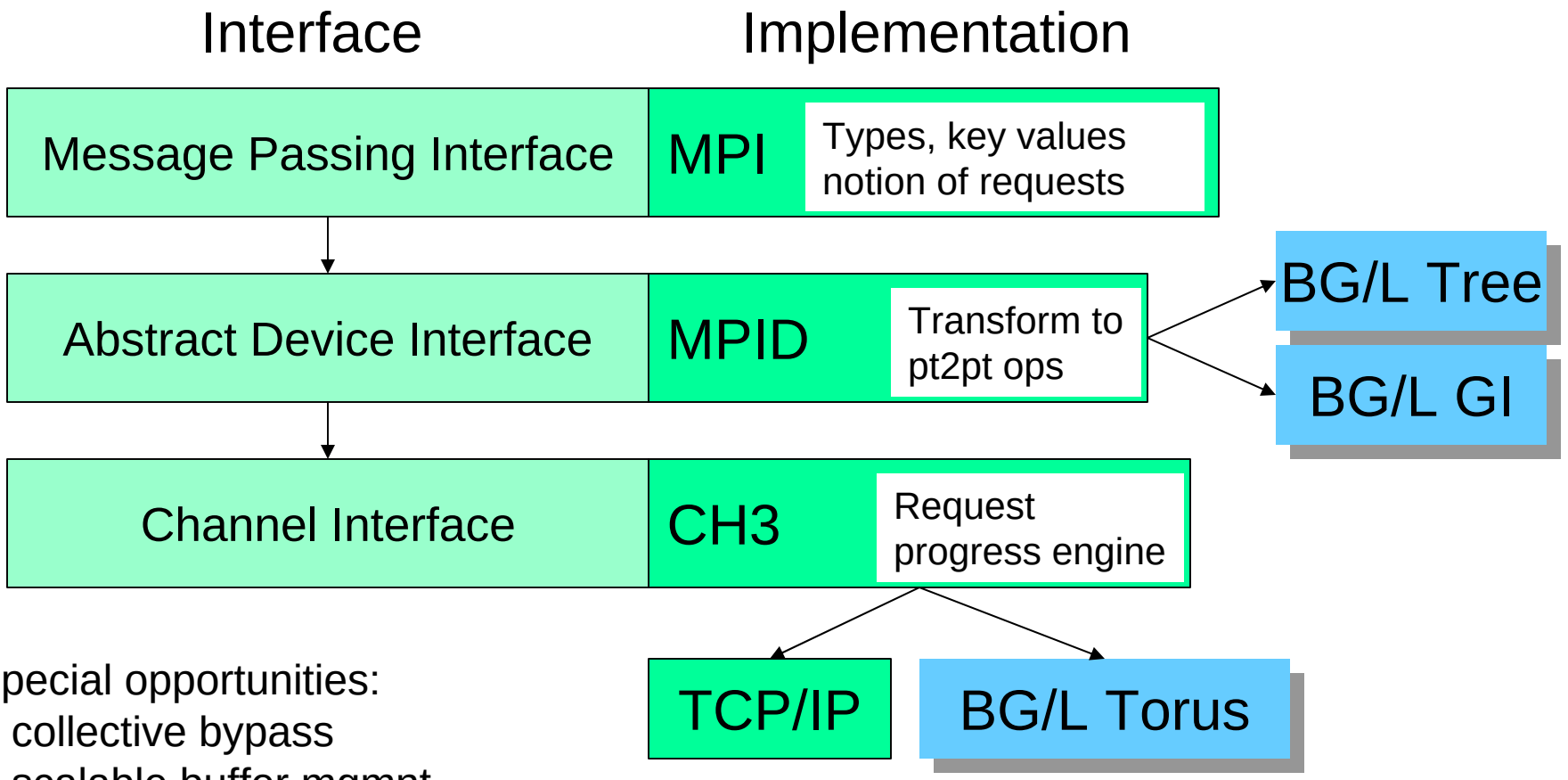
- Pollable and active-message data paths
- RMA Path

Early Results on Channel/TCP Device



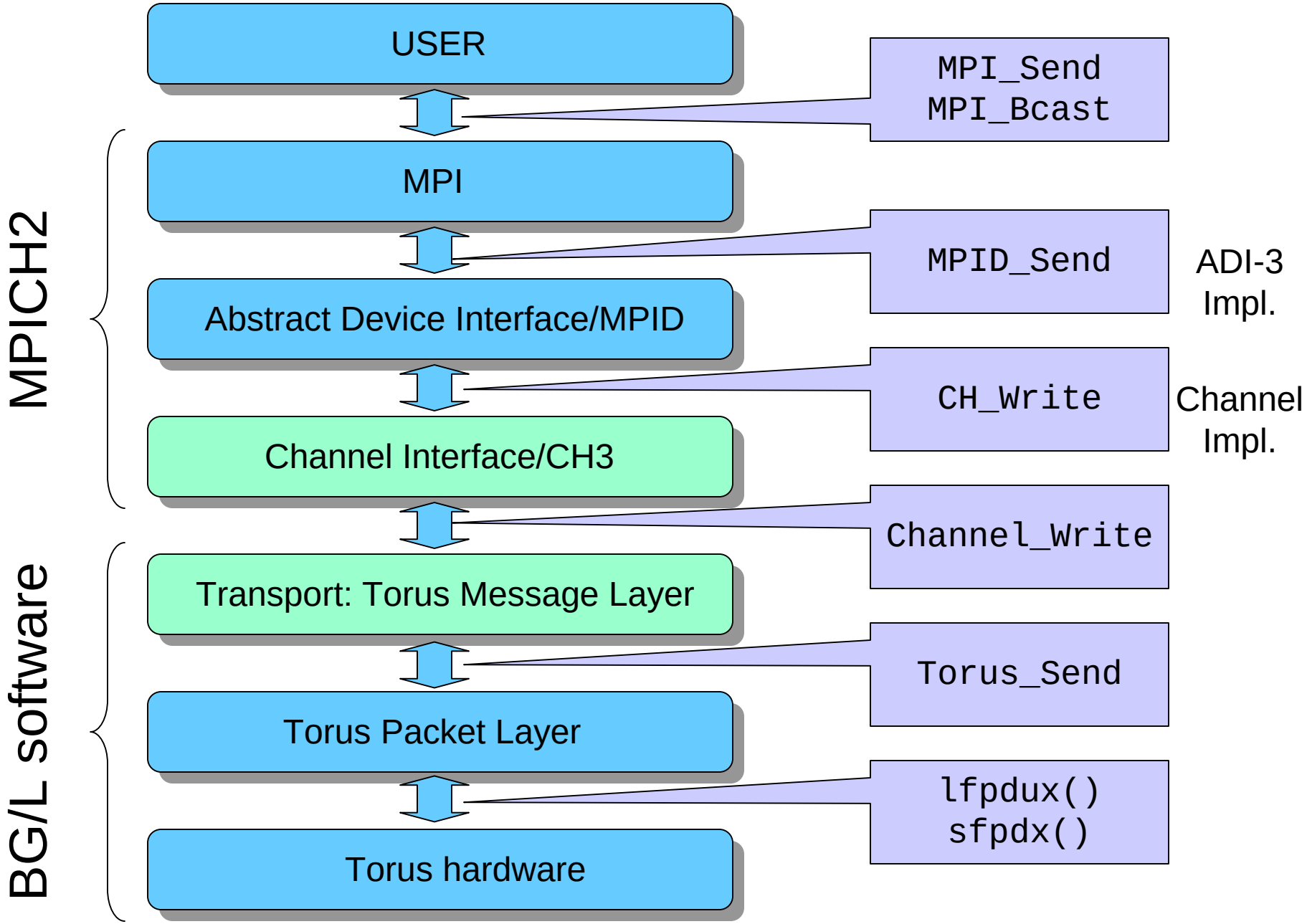
- Conclusion: little added overhead over low-level communication
  - But will become more critical with high-performance network

BG/L and the MPICH2 Architecture



Special opportunities:

- collective bypass
- scalable buffer mgmnt
- out-of-order network


USER
MPI
Abstract Device Interface/MPID
Channel Interface/CH3
Transport: Torus Message Layer
Torus Packet Layer
Torus hardware
MPICH2
BG/L software
MPI_Send
MPI_Bcast
MPID_Send
ADI-3
Impl.
CH_Write
Channel
Impl.
Channel_Write
Torus_Send
lfpdux()
sfpdx()

Some Questions That You Are About to Ask

- Out-of-order delivery of packets in the network
  - Channel device enhanced to simplify support
  - Few MPI communications require ordering; channel supports ordering of message headers to enable message tracing tools such as Jumpshot
- Implementation of collectives without MPI point-to-point (e.g., using the other network)
  - Improved version of mechanism used in MPICH-1 (introduced for the Meiko) allows each collective operation to use special routines on a communicator-by-communicator basis
- Scalable eager buffer and connection management
  - Dynamic buffer allocation and connection management is consistent with the ADI design (virtual connection table, currently an array, can be replaced with a sparse array).
- Polling and non-polling
  - Design supports both. Neither is always best.

Some More Questions

- Thread safety
  - Careful use of atomic operations avoids locks in many cases. Both configure-time and runtime control of the level of thread safety. All versions support OpenMP-style loop parallelism
- Process(or) topology
  - Interface through MPI_Cart_create and MPI_Graph_create
- RMA (one-sided)
  - Design uses operation aggregation to eliminate extra operations and access windows to eliminate serialization present in other implementations of MPI RMA
- Rendezvous optimizations
  - Single communication method case can use an “unexpected receive” approach, already used in some prototype MPI implementations, to avoid one handshake message

Another Question

- How to best use the second CPU?
  - Multiple modes possible
    - 2nd CPU idle (“heater” mode)
    - 2nd CPU runs 2nd thread in same MPI process (“symmetric” mode)
      - At least initially
      - Exploring using for 2nd MPI process (“virtual node” mode)
    - 2nd CPU acts as communication co-processor
      - Allows true overlap of computation and communication
      - Allows peak performance
        - “middle packet” optimization
  - Current plan: support all modes

MPI in BG/L: Using the 2nd CPU

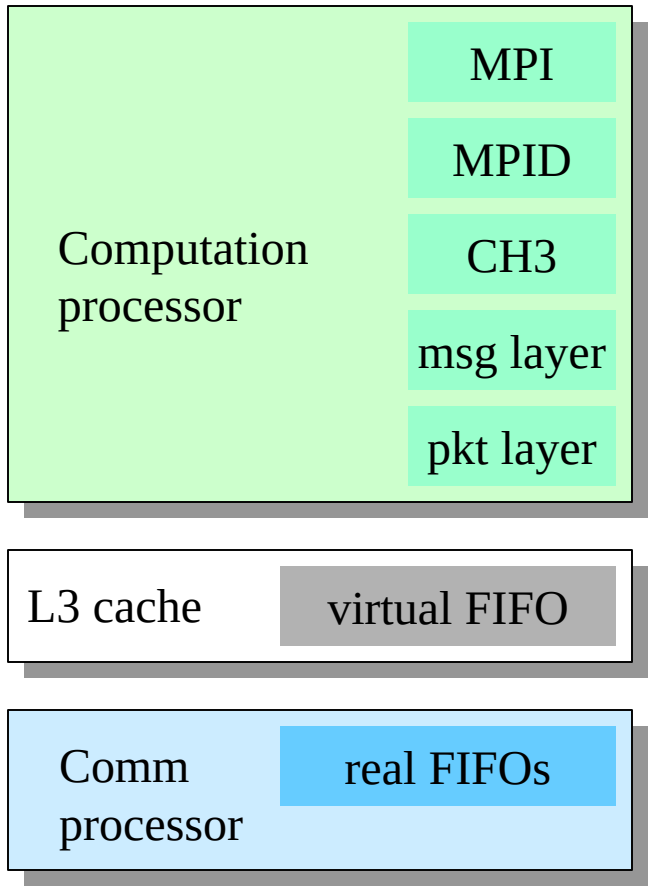
- Processing modes:
  - heater mode
  - symmetric
    - 1 MPI rank per ASIC
  - *communication co-processor*
- Compute processor:
  - post, allocate, match graduate MPI requests
  - progress at channel protocol level
- Comm. processor:
  - progress at transport level
    - packets
    - messages

Ground Rule #1:

MPI primitives are executed by compute processor

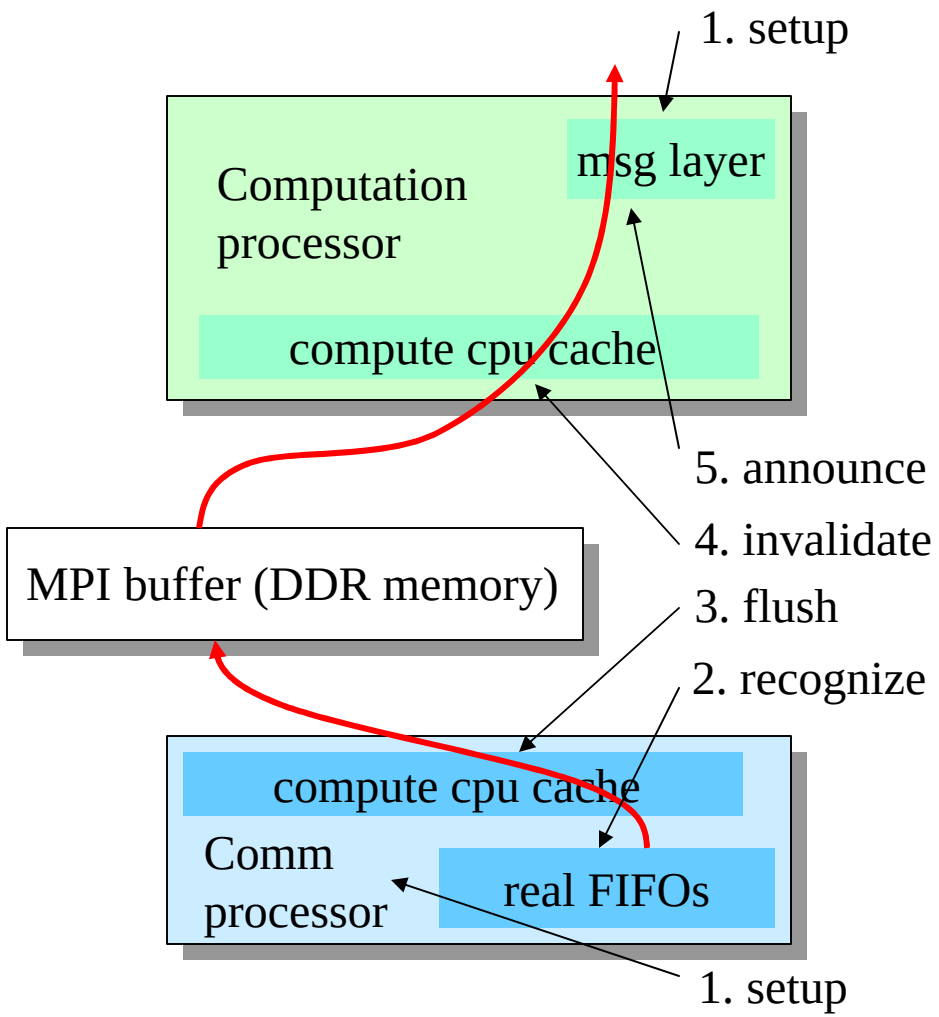
Communication co-processor

- co-processor looks like a **big** *virtual* torus device
  - **+** high performance
  - **+** no coherency problem
  - **+** compatible
  - **+** perfect for a first cut
  - **-** latency
  - **-** can do better



“Middle packet” optimization

- aligned packets of matched/allocated requests
- coprocessor streams to/from request buffers
  - + truly 0-copy
  - + good latency
  - + true comm. overlap
  - - needs co-ordination
  - - fragile
  - - only for aligned packets



Status of BG/L MPI Implementation Today

- Running (!) in
  - Emulation
    - native Linux/IA32
    - 2:1 slowdown
  - Simulation
    - Linux/**`bglsim`**
    - ~10^3 slowdown
- Message Layer supports CH3 “eager protocol”
  - Does not yet provide correct inter-message ordering
  - Does not implement optimistic error control
  - Does not yet have specialized collective operations
  - MPICH-2 does not yet have all of MPI, but:
- NAS parallel benchmarks
  - experiments on 2 to 4 processors

Process Manager Research Issues

- Identification of proper process manager functions
  - Starting (with arguments and environment), terminating, signaling, handling stdio, …
- Interface between process manager and communication library
  - Process placement and rank assignment
  - Dynamic connection establishment
  - MPI-2 functionality: Spawn, Connect, Accept, Singleton Init
- Interface between process manager and rest of system software
  - Cannot be separated from system software architecture in general
  - Process manager is important component of component-based architecture for system software, communicating with multiple other components
- Scalability
  - A problem even on existing large systems
  - BG/L presents new challenges

Process Manager Research at ANL

- MPD – prototype process management system
- Original Motivation: faster startup of interactive MPICH programs
- Evolved to explore general process management issues, especially in the area of communication between process manager and parallel library
- Laid foundation for scalable system software research in general
- MPD-1 is part of current MPICH distribution
  - Much faster than earlier schemes
  - Manages stdio scalably
  - Tool-friendly (e.g. supports TotalView)

Requirements on Process Manager from Message-Passing Library

- Individual process requirements
  - Same as for sequential job
  - To be brought into existence
  - To receive command-line arguments
  - To be able to access environment variables
- Requirements derived from being part of a parallel job
  - Find size of job: MPI_Comm_size(MPI_COMM_WORLD, &size)
  - Identify self: MPI_Comm_rank(MPI_COMM_WORLD, &myrank)
  - Find out how to contact other processes: MPI_Send(…)

Finding the Other Processes

- Need to identify one or several ways of making contact
  - Shared memory (queue pointer)
  - TCP (host and port for connect)
  - Other network addressing mechanisms (Infiniband)
  - (x,y,z) torus coordinates in BG/L
- Depends on target process
- Only process manager knows where other processes are
- Even process manager might not know everything necessary (e.g. dynamically obtained port)
- “Business Card” approach

Approach

- Define interface from parallel library (or application) to process manager
  - Allows multiple implementations
  - MPD is a scalable implementation (used in MPICH ch_p4mpd device)
- PMI (Process Manager Interface)
  - Conceptually: access to spaces of key=value pairs
  - No reserved keys
  - Allows very general use
  - Basic part: for MPI-1, other simple message-passing libraries
  - Advanced part: multiple keyval spaces for MPI-2 functionality, grid software
- Provide scalable PMI implementation with fast process startup
- Let others do so too

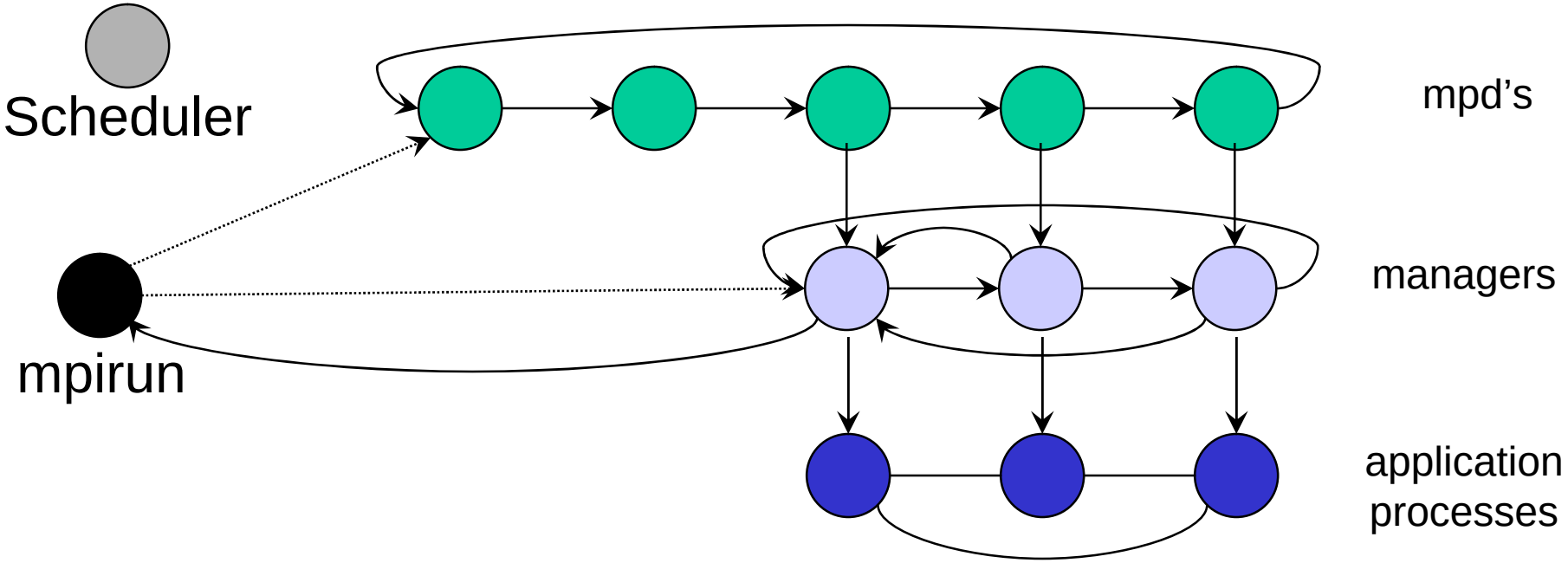
The PMI Interface

- PMI_Init
- PMI_Get_size
- PMI_Get_rank
- PMI_Put
- PMI_Get
- PMI_Fence
- PMI_End

- More functions for managing multiple keyval spaces
  - Needed to support MPI-2, grid applications

MPD

Architecture of MPD:



Interesting Features

- Security
  - “Challenge-response” system, using passwords in protected files and encryption of random numbers
  - Speed not important since daemon startup is separate from job startup
- Fault Tolerance
  - When a daemon dies, this is detected and the ring is reknit => minimal fault tolerance
  - New daemon can be inserted in ring
- Signals
  - Signals can be delivered to clients by their managers

More Interesting Features

- Uses of signal delivery
  - signals delivered to a job-starting console process are propagated to the clients
    - so can suspend, resume, or kill an mpirun
  - one client can signal another
    - can be used in setting up connections dynamically
  - a separate console process can signal currently running jobs
    - can be used to implement a primitive gang scheduler
- Mpirun also represents parallel job in other ways

  totalview mpirun –np 32 a.out

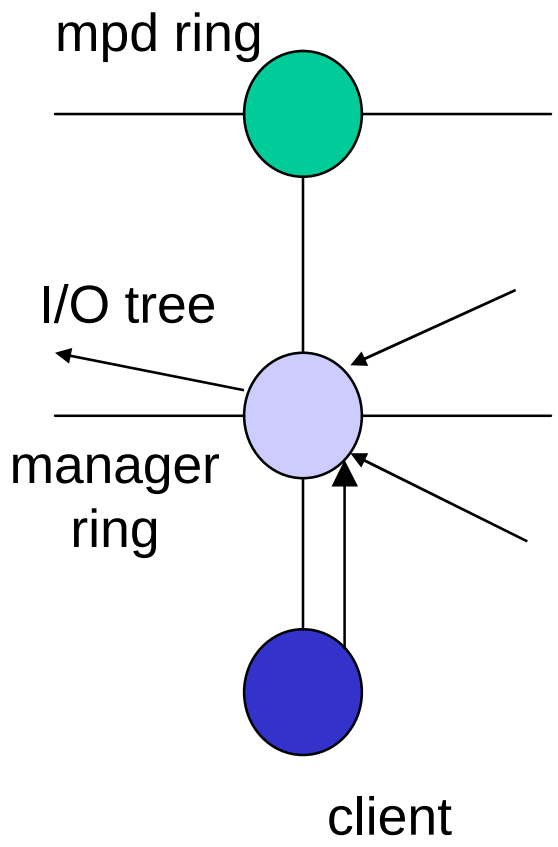
  runs 32-process job under TotalView control

More Interesting Features

- Support for parallel libraries
  - implements the PMI process manager interface, used by MPICH.
    - groups, put, get, fence, spawn
    - simple distributed database maintained in the managers
    - solves “pre-communication” problem of startup
    - makes MPD independent from MPICH while still providing needed features

Handling Standard I/O

- Managers capture **`stdout`** and **`stderr`** (separately) from their clients
- Managers forward **`stdout`** and **`stderr`** (separately) up a pair of binary trees to the console, optionally adding a rank identifier as line label
- Console's **`stdin`** is delivered to **`stdin`** of client 0 by default, but can be controlled to broadcast or go to specific client



The Scalable Systems Software SciDAC Project

- Multiple Institutions (most national labs, plus NCSA)
- Targeting systems software for large systems, particularly clusters
- Component architecture
- Currently using XML for inter-component communication
- Status
  - Early demos; watch for more at SC'02, some components in use at Argonne on Chiba City cluster
  - Detailed XML interface to PM component, implemented by MPD
- One powerful effect: forcing rigorous (and aggressive) definition of what a process manager should do and what should be encapsulated in other components
  - Start (with arguments and environment variables), terminate, cleanup
  - Signal delivery
  - Interactive support (e.g. for debugging) – requires stdio management

What Does This Have to Do with MPI on BGL?

- MPI library needs PMI interface implementation
- LoadLeveler desirable as scheduler
  - It exists!
  - Provides sophisticated scheduling capabilities
  - Familiar to large class of users
- LoadLeveler can be used as scheduling component in Scalable System Software Center sense
  - Interface to process manager well defined
  - Interface has needed features
  - MPD-based process manager ready for use
  - Currently collaborating with IBM/Haifa group on this approach to scheduling and process management for BG/L
- LoadLeveler only one option for scheduling component
  - Clear definitions of interfaces will support use of other schedulers
    - (e.g., SLURM)

MPD Supports Multiple Styles of Process Management

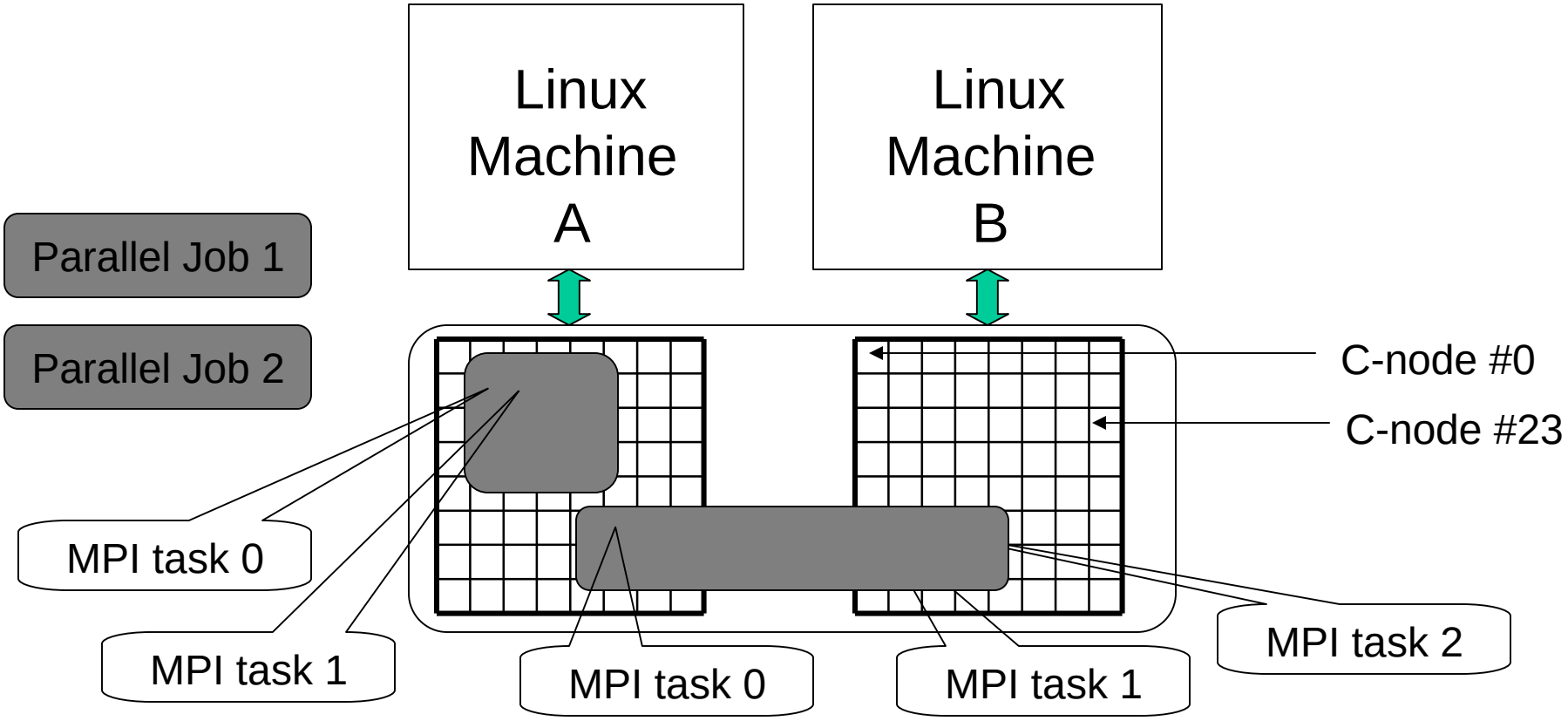
- Scheduler can compose and execute mpirun command that communicates with MPD ring
  - Easy to write BG/L-specific mpirun scripts
    - (e.g. to specify topology information)
- Scheduler can communicate directly with mpd ring
- Scheduler, other components of system software can communicate with persistent process manager component, using public XML interface
- Scheduler can allocate nodes for interactive use and user can run mpirun interactively
  - (e.g. for debugging)
- User can set up own MPD ring in user mode
  - (e.g. for development)

LoadLeveler and MPD for BG/L

- Goals
  - Provide functional and familiar job submission, scheduling, and process management environment on BG/L
  - Change existing code base (LL, MPICH, MPD) as little as possible
- Current Plan: Run MPD's as root and have LL submit job to MPD's to start user job as user
- LL can schedule set of nodes for user to use interactively; then user can use mpirun to run series of short interactive jobs on subsets of allocated nodes
  - Ensure that user can only use scheduled nodes
- Build foundation for development of other scheduling and process management approaches

BG/L Architecture

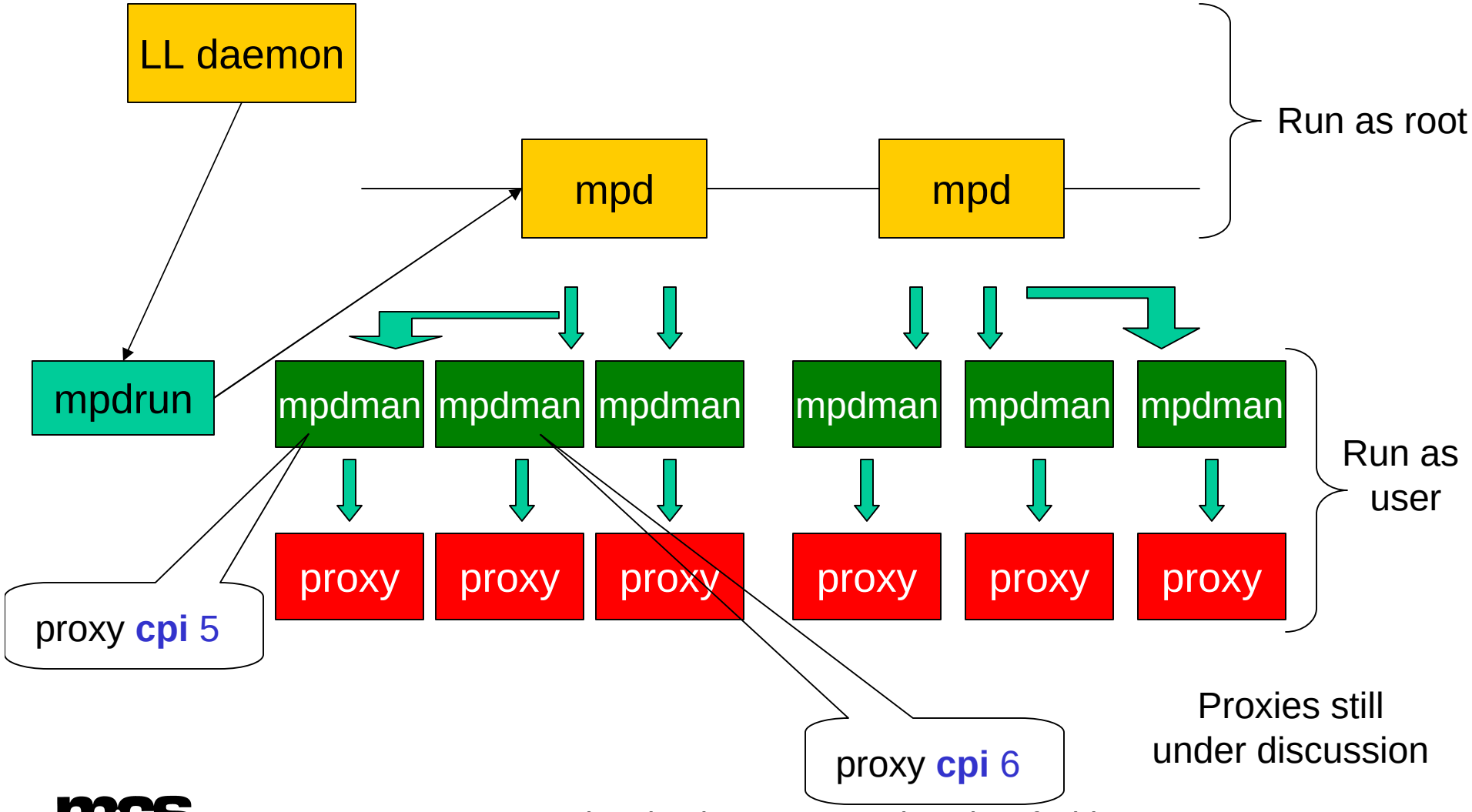
- Example : 2 I/O nodes, each with 64 compute nodes



Proxy processes

- A proxy process (Linux process) is created for each MPI task
- The task is not visible to the operating-system scheduler
- The proxy interfaces between the operating-system and the task, passing signals, messages etc…
- It provides transparent communication with the MPI task
- MPD will start these proxy processes
  - Need to be able to pass separate arguments to each

Running the Proxies on the Linux Nodes



Conclusion

- IBM and ANL are collaborating in two related areas to improve the usability of BG/L
  - MPI implementation
  - Process management
- In each case timing seemed to be perfect to connect existing research projects to new scalability challenges
- Early results are promising